Entropy production in classical and quantum systems

Claude-Alain Pillet

Entropy production in classical and quantum systems

CLAUDE-ALAIN PILLET

CPT-CNRS Luminy, Marseille, France
Université de Toulon et du Var, La Garde, France

Abstract. Koopmanism – the spectral theory of dynamical systems – reduces the study of dynamical properties of a classical or quantum system $\mathcal{S}$ to the spectral analysis of its Liouvillean $L_{\mathcal{S}}$. By definition, the operator $L_{\mathcal{S}}$ implements the dynamics on a suitable representation of the observable algebra of $\mathcal{S}$. Near thermal equilibrium, this representation can often be constructed explicitely. Recent developments have shown that, in this situation, spectral analysis becomes a powerful tool in the study of thermal relaxation processes. Far from thermal equilibrium, the explicit construction of stationary states and of the corresponding representations is usually not possible. Nevertheless, important physical properties of the system $\mathcal{S}$ can be obtained from a fairly simple mathematical analysis. In this work, I investigate entropy production in open systems driven away from equilibrium by thermodynamic forces.

Keywords. Nonequilibrium statistical mechanics, open systems, Hamiltonian systems, entropy production, Koopmanism.

PACS. 05.20.-y, 05.30.-d, 05.45.-a, 05.70.Ln, 31.70.Hq, 44.10.+i.

1 Introduction

Important efforts have recently been focussed on the rigorous development of nonequilibrium statistical mechanics. Roughly speaking we can distinguish two main streams in this growing body of works:

- **Thermostated systems.** A Hamiltonian system Σ, with a large but finite number of degrees of freedom, is driven away from equilibrium by non-hamiltonian and/or time dependent forces and constrained to a compact energy surface by a Gaussian thermostat.

- ► **Open systems.** The same system Σ is allowed to interact with infinite reservoirs $\mathcal{R}_1$,$\mathcal{R}_2$, ..., $\mathcal{R}_n$, the coupled system $\mathcal{S} = \Sigma + \mathcal{R}_1 + \cdots$ remaining Hamiltonian.

In both cases nonequilibrium states of the system Σ (also called dynamical ensembles) are obtained as weak limits, under time evolution, of appropriate initial states. From a methodological point of view, these two ways of defining a dynamics on Σ should be understood as two different schemes modelizing the same physical situation. More precisely, the *thermostat vs. reservoir* alternative generalizes to nonequilibrium the *microcanonical vs. canonical* (or grand canonical) ensembles of equilibrium statistical mechanics. We expect that, as Σ becomes large, the dynamical ensembles defined by the two dynamics become equivalent. We are still far from a precise formulation of this extended equivalence principle. However, see [R5] and references therein for related results.

Recent investigations of thermostated systems are based on the «chaotic hypothesis» of Gallavotti and Cohen [CG], an adaptation of the «Ruelle principle» of turbulent fluid dynamics [R1]. In the spirit of Boltzmann's ergodic hypothesis, the dynamics of Σ is *assumed* to be strongly chaotic (uniformly hyperbolic). Under the chaotic hypothesis, dynamical ensembles can be identified with SRB measures. This fact brings the powerful machinery of Axiom A systems into the game. The reader can find an excellent survey of this subject in [R3].

The fact that there is no natural way to quantize thermostated systems makes the alternative approach trough open systems unavoidable in quantum statistical mechanics. From a more philosophical point of view, a unified treatment of classical and quantum nonequilibrium dynamics requires the parallel development of a classical theory of open systems. Recent results in these directions can be subdivided in three classes according to the initial state of the reservoirs.

If there is only one reservoir $\mathcal{R}$ at thermal equilibrium, thermodynamic stability requires the full system $\mathcal{S} = \Sigma + \mathcal{R}$ to approach thermal equilibrium with the same values of intensive parameters. This has been proved for quite general classical Hamiltonian systems Σ coupled to a harmonic radiation field $\mathcal{R}$ in [JP1]. The first quantum mechanical result can be found in [JP2], where return to equilibrium of the spin-boson model (a 2-level atom coupled to a free boson field) at high temperature is proved. More recently, this result has been extended to a N-level atom coupled to the electromagnetic field at arbitrary temperature in [BFS]. For further extensions to more general Pauli-Fierz systems, see [DJ] and [DJP].

If the system Σ is coupled to several reservoirs in thermal equilibrium at different temperatures, one expects the corresponding dynamical ensembles to describe a steady heat flow trough the system. In this situation, the first mathematical problem is the existence of dynamical ensembles. This question was considered in [EPR1], where the existence of a steady state is proved for a finite chain of classical, weakly anharmonic oscillators coupled at its two ends to reservoirs $\mathcal{R}_1$ and $\mathcal{R}_2$. The unicity and mixing property of this stationary state are proved in [EPR2], where the existence of a steady heat flow through the system is also established. More recently, these results have been extended to the strongly anharmonic regime in [EH]; moreover a detailed study of the asymptotic behavior of the stationary state at low temperature can be found in [RT].

Finally, the system Σ can also be driven away from thermal equilibrium if the reservoirs themselves are initially far from equilibrium. In [FL], weakly anharmonic perturbations of an infinite quantum harmonic chain are considered. A large family of quasi-free, nonequilibrium stationary states of the chain is proved to be stable under local perturbations, providing a wealth of nonequilibrium states for the anharmonic chain. In a more axiomatic setup, under a strong ergodicity assumption, natural nonequilibrium states for a N-level atom coupled to several reservoirs and subject to external time-dependent forces are constructed in [R4]. The linear response formula is also proved to remain valid far from equilibrium.

Many of the above results on open systems have been proved by first constructing a «normal form» of the system, *i.e.* a distinguished representation of its algebra of observables in a Hilbert space where the dynamics is implemented by a unitary group $U_t = \mathrm{e}^{-iLt}$, and the stationary state by a unit vector Ω. In such a representation, ergodic properties of the system can be obtained from spectral and scattering theory of the self-adjoint generator L. For example, return to equilibrium follows from the fact that L has purely absolutely continuous spectrum, except for a simple eigenvalue at 0.

This circle of ideas is well known in the ergodic theory of dynamical systems, going under the name «Koopmanism». At or near thermal equilibrium, the normal form can often be constructed explicitely since we have a good candidate for the stationary state: The classical or quantum Gibbs Ansatz. This explains the success of the method in this regime. Far from equilibrium the stationary state is not explicitely known. It is constructed as a weak limit, under the time evolution, of suitable initial states. Moreover it is singular with respect to these initial states (technically, its normal form live in a different folium of representations).

In this paper I adopt a somewhat different point of view, and work in the normal form associated with the initial state. For a large class of models describing a small system Σ driven away from equilibrium by temperature gradients, I define entropy production and show that it is non-negative. I also describe the relation between entropy production and the heat currents flowing through the system.

The paper is organized as follows. Section 2 is a brief survey of the normal forms of the simple systems which will be the building blocks of our open system $\mathcal{S}$. Section 3 introduces the technical tool used in this paper: the modular structure of normal forms. In Section 4, I define the model, and prove that its entropy production is non-negative.

2 Normal Forms

Definition 1 The system $\mathcal{S}$ is in normal form if it is described by a Hilbert space $\mathcal{H}$, a von Neumann algebra $\mathfrak{M} \subset \mathcal{B}(\mathcal{H})$, a unit vector $\Omega \in \mathcal{H}$ and a self-adjoint operator L on $\mathcal{H}$ with the following properties.

(a) Ω is cyclic for $\mathfrak{M}$: $\overline{\mathfrak{M}\Omega} = \mathcal{H}$.

(b) Ω is separating for $\mathfrak{M}$: $X \in \mathfrak{M}$, $X\Omega = 0 \Rightarrow X = 0$.

(c) $L\Omega = 0$.

(d) $\mathrm{e}^{iLt}\mathfrak{M}\mathrm{e}^{-iLt} = \mathfrak{M}$ for all $t \in \mathbb{R}$.

The algebra $\mathfrak{M}$ is the set of observables of $\mathcal{S}$. The operator L, the Liouvillean of $\mathcal{S}$, generates the dynamics on $\mathfrak{M}$: $\tau^t(X) = \mathrm{e}^{iLt}X\mathrm{e}^{-iLt}$. The vector Ω defines the stationary state: $\mathfrak{M} \ni A \mapsto \omega(X) = (\Omega, X\Omega)$.

The normal form is unique, up to unitary equivalence. If the system $\mathcal{S}$ decomposes into non-interacting subsystems, $\mathcal{S} = \sum_\alpha \mathcal{S}_\alpha$, its normal form is the tensor product of the normal forms of its components: $\mathcal{H} = \otimes_\alpha \mathcal{H}_\alpha$, ... There is a completely general method to bring a system into its normal form: The GNS construction. However, this is a rather abstract construction. The following examples display explicit representations of the normal form of systems with a finite number of degrees of freedom. They will play the role of Σ in our model.

Example 2 A classical Hamiltonian system with finite dimensional phase space G, Poisson bracket $\{\cdot,\cdot\}$, Hamiltonian H and invariant measure μ has a normal form given by: $\mathcal{H} = L^2(G, d\mu)$, $\mathfrak{M} = L^\infty(G, d\mu)$, $\Omega = 1$ and $L = i\{H, \cdot\}$. The group generated by L is $\mathrm{e}^{iLt}f = f \circ \Phi_H^t$, where Φ_H is the Hamiltonian flow generated by H on G. Thermal equilibrium at inverse temperature β corresponds to $d\mu = Z_\beta^{-1}\mathrm{e}^{-\beta H}d\ell$ where ℓ is the Liouville measure on G.

Example 3 Let $\mathcal{S}$ be a quantum system with finitely many degrees of freedom, Hilbert space $\mathfrak{h}$, Hamiltonian H and density matrix $\rho = \sum_n p_n |\varphi_n >< \varphi_n|$. Assuming $\rho > 0$ and $[H, \rho] = 0$, the normal form of $\mathcal{S}$ is given by: $\mathcal{H} = \mathfrak{h} \otimes \mathfrak{h}$, $\mathfrak{M} = \mathcal{B}(\mathfrak{h}) \otimes I$, $\Omega = \sum_n p_n^{1/2}\varphi_n \otimes \varphi_n$ and $L = H \otimes I - I \otimes H$. Thermal equilibrium at inverse temperature β corresponds to $\rho = Z_\beta^{-1}\mathrm{e}^{-\beta H}$.

Thermal equilibrium of systems with infinitely many degrees of freedom is most conveniently characterized by the KMS condition.

Definition 4 A quantum system $\mathcal{S}$, in normal form, is in thermal equilibrium at inverse temperature β if there exists a σ-weakly dense τ-invariant $*$-subalgebra $\mathfrak{U}_\beta \subset \mathfrak{M}$, such that

- $\mathfrak{U}_\beta\Omega \subset \mathrm{D}(\mathrm{e}^{-\beta L/2})$;
- $(\mathrm{e}^{-\beta L/2}X\Omega, \mathrm{e}^{-\beta L/2}Y\Omega) = (Y^*\Omega, X^*\Omega)$ for $X, Y \in \mathfrak{U}_\beta$.

See [BR2] for a more general definition and a complete discussion of the quantum KMS condition. For a classical system $\mathcal{S}$, the symplectic structure of phase space induces a Poisson bracket $\{\cdot, \cdot\}$ on sufficiently «regular» observables.

Definition 5 A classical system $\mathcal{S}$, in normal form, is in thermal equilibrium at inverse temperature β if there exists a σ-weakly dense τ-invariant $*$-subalgebra $\mathfrak{U}_\beta \subset \mathfrak{M}$, such that

- $\mathfrak{U}_\beta\Omega \subset \mathrm{Q}(L)$ (the form domain of L);
- $\beta(X\Omega, LY\Omega) = (\Omega, i\{X^*, Y\}\Omega)$ for $X, Y \in \mathfrak{U}_\beta$.

See [A1] and [A2] for a detailed study of the classical KMS condition.

Notation. Let $\mathfrak{h}$ be a complex Hilbert space. $\Gamma(\mathfrak{h})$ denotes the symmetric Fock space over $\mathfrak{h}$. For $f \in \mathfrak{h}$, $a^*(f)$ and $a(f)$ are the associated creation and annihilation operators and $\phi(f) = \frac{1}{\sqrt{2}}(a^*(f) + a(f))$ is the Segal field operator. If A is an operator on $\mathfrak{h}$, $d\Gamma(A)$ denotes its second quantization.

The following examples give the normal form of infinite systems wich will play the role of the reservoirs $\mathcal{R}_\alpha$ in our model.

Example 6 A classical harmonic field is an infinite dimensional Hamiltonian system whose phase space is a real Hilbert space $\mathfrak{h}$ with the symplectic structure induced by a non-singular skew-adjoint operator l [1]. The Hamiltonian is $H(\phi) = \frac{1}{2}\|\phi\|^2$, and the flow it generates on $\mathfrak{h}$ is the unitary group e^{lt}.

> For example, the classical scalar wave-field on $\mathbb{R}^3$ whose dynamics is given by the wave equation $\ddot{\varphi} = \Delta\varphi$ is described by the Hilbert space of real functions
> $$\phi(x) = \begin{pmatrix} \varphi(x) \\ \pi(x) \end{pmatrix},$$
> with the norm $\|\phi\|^2 = \int (|\nabla\varphi|^2 + \pi^2)\, dx$ and the symplectic structure induced by
> $$l = \begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}.$$

The thermal equilibrium state at inverse temperature β of a classical harmonic field is the Gaussian measure with covariance $\beta^{-1}(\cdot,\cdot)$. The normal form associated with this state is given by: $\mathcal{H} = \Gamma(\mathfrak{h}_{\mathbb{C}})$, where $\mathfrak{h}_{\mathbb{C}}$ is the complexification of $\mathfrak{h}$. Ω is the Fock vacuum. $\mathfrak{M}$ is the commutative von Neumann algebra generated by the family $\{\mathrm{e}^{i\phi_\beta(f)} | f \in \mathfrak{h}\}$, where $\phi_\beta(f) = \beta^{-1/2}\phi(f)$ are canonical field operators, and $L = id\Gamma(l)$.

Example 7 The normal form of a free, scalar, Bose field in $\mathbb{R}^3$, at thermal equilibrium (without condensate) at inverse temperature β is given by the Araki-Woods representation [AWo]: $\mathcal{H} = \Gamma(\mathfrak{h}) \otimes \Gamma(\mathfrak{h})$, where $\mathfrak{h} = L^2(\mathbb{R}^3)$ is the one-particle Hilbert space. $\Omega = \Omega_F \otimes \Omega_F$, where Ω_F is the Fock vacuum. $L = d\Gamma(h) \otimes I -$

[1] *i.e.*, the Poisson bracket is $\{F, G\} = (\nabla F, l\nabla G)$.

$I \otimes d\Gamma(h)$, where h is the one particle Hamiltonian. With $\rho = (\mathrm{e}^{\beta h} - 1)^{-1}$, $\mathfrak{M}$ is the von Neumann algebra generated by the family $\{\mathrm{e}^{i\phi_\rho(f)} | f \in \mathrm{D}(\rho^{1/2})\}$, where $\phi_\rho(f) = \phi(\sqrt{1+\rho} f) \otimes I + I \otimes \phi(\sqrt{\rho}\bar{f})$ is the Araki-Woods field operator. A similar representation exists for fermions [AWy].

Example 8 The normal form of a classical ideal gas of identical particles of mass m in $\mathbb{R}^3$ is given by: $\mathcal{H} = \Gamma(\mathfrak{h})$, where $\mathfrak{h} = L^2(\mathbb{R}^3 \times \mathbb{R}^3, dq\, dp)$. Ω is the Fock vacuum and $L = id\Gamma(p/m \cdot \nabla_q)$. $\mathfrak{M}$ is the commutative von Neumann algebra generated by the family $\{\mathrm{e}^{iN_\rho(f)} | f \in C_0^\infty(\mathbb{R}^3 \times \mathbb{R}^3)\}$, where

$$N_\rho(f) = \int f(q,p)(a^*(q,p) + \sqrt{\rho(p)})(a(q,p) + \sqrt{\rho(p)}) dq\, dp,$$

and $\rho(p) = (2\pi m/\beta)^{-3/2} \mathrm{e}^{-\beta p^2/2m}$ is the Maxwell distribution.

3 Modular structures

The main advantage of the normal form of a system $\mathcal{S}$ is the existence of a rich mathematical structure which, in the quantum case, brings the modular theory of von Neumann algebra into the playground. In the classical case, this structure is far less understood. In this section I briefly recall the basics of modular theory and its relation to statistical mechanics.

3.1 Quantum KMS states and Tomita-Takesaki theory

Let $\mathcal{S} = (\mathcal{H}, \mathfrak{M}, \Omega, L)$ be a quantum system in normal form. The densely defined anti-linear involution

$$\begin{array}{rcl} \mathfrak{M}\Omega & \rightarrow & \mathcal{H} \\ X\Omega & \mapsto & X^*\Omega \end{array}$$

has a closure S such that, for any $\Psi \in \mathrm{D}(S)$, there exists a closed operator C, affiliated to $\mathfrak{M}$, with $\Psi = C\Omega$ and $S\Psi = C^*\Omega$. The polar decomposition of S, written as $S = J\mathrm{e}^{\mathcal{L}/2}$, defines an anti-unitary operator J called the modular conjugation and a self-adjoint operator $\mathcal{L}$ called the modular generator. It follows easily from these definitions that J is an involution ($J^2 = I$) which anti-commutes with $\mathcal{L}$: $J\mathcal{L} + \mathcal{L}J = 0$. Moreover, the adjoint $S^* = J\mathrm{e}^{-\mathcal{L}/2}$ is characterized by $\mathcal{S}^* X\Omega = X^*\Omega$ for any $X \in \mathfrak{M}'$. These objects define an involution j and a group of automorphisms σ^t on $\mathcal{B}(\mathcal{H})$ via the formulae

$$\begin{array}{rcl} j(X) & = & JXJ, \\ \sigma^t(X) & = & \mathrm{e}^{it\mathcal{L}} X \mathrm{e}^{-it\mathcal{L}}. \end{array}$$

The Tomita-Takesaki Theorem states that

$$\begin{array}{rcl} j(\mathfrak{M}) & = & \mathfrak{M}', \\ \sigma^t(\mathfrak{M}) & = & \mathfrak{M}, \end{array}$$

so that, in particular, σ^t defines an automorphism of $\mathfrak{M}$ which is called the modular group of $\mathfrak{M}$. This group commutes with the dynamics, *i.e.*,

$$[\mathcal{L}, L] = 0.$$

Moreover, Takesaki's Theorem states that σ is the only dynamics on $\mathfrak{M}$ for which ω is a KMS state at temperature -1. It follows immediately that $\mathcal{S}$ is at thermal equilibrium at inverse temperature β if and only if

$$\mathcal{L} = -\beta L, \tag{1}$$

(compare with the KMS condition in Section 2. See [BR1] for details and proofs).

Another important object associated with the modular structure is the natural cone

$$\mathcal{P} \equiv \overline{\mathrm{e}^{\mathcal{L}/4}\mathfrak{M}_+\Omega} = \overline{\{Xj(X)\Omega | X \in \mathfrak{M}\}},$$

where $\mathfrak{M}_+$ denotes the set of positive elements of $\mathfrak{M}$. For any normal state μ on $\mathfrak{M}$, there is a unique unit vector $\Omega_\mu \in \mathcal{P}$ such that $\mu(X) = (\Omega_\mu, X\Omega_\mu)$ for all $X \in \mathfrak{M}$. Moreover, μ is faithful $\Leftrightarrow$ Ω_μ is separating for $\mathfrak{M}$ $\Leftrightarrow$ Ω_μ is cyclic for $\mathfrak{M}$. If μ and ν are two faithful normal states on $\mathfrak{M}$, the densely defined anti-linear map

$$\begin{array}{rcl} \mathfrak{M}\Omega_\nu & \to & \mathfrak{M}\Omega_\mu \\ X\Omega_\nu & \mapsto & X^*\Omega_\mu \end{array}$$

has a closure $S_{\mu|\nu}$. Its polar decomposition, written as $S_{\mu|\nu} = J_{\mu|\nu}\Delta_{\mu|\nu}^{1/2}$, defines a positive operator $\Delta_{\mu|\nu}$ called relative modular operator.

3.2 Classical KMS states and Gallavotti-Pulvirenti modular structure

Due to the abelian nature of the algebra $\mathfrak{M}$, the Tomita-Takesaki modular theory is trivial for a classical system. It was first noticed in [GP] that, under suitable regularity conditions on the state ω, another structure exists in this case. Its relation with Tomita-Takesaki theory is probably best understood by considering the classical limit of a quantum system. Instead, I shall take Takesaki's Theorem as a starting point.

Definition 9 The state of the classical system $\mathcal{S} = (\mathcal{H}, \mathfrak{M}, \Omega, L)$ is regular if there exists a unique Hamiltonian flow σ^t on $\mathfrak{M}$ for which it is an equilibrium state a temperature -1.

By the classical KMS condition, $\mathcal{S}$ is in a regular state if there exists a self-adjoint operator $\mathcal{L}$ and a σ-weakly dense $*$-subalgebra $\mathfrak{U} \subset \mathfrak{M}$ such that $\mathcal{L}$ is essentially self-adjoint on $\mathfrak{U}\Omega$, and

$$(\Omega, i\{X^*, Y\}\Omega) = -(X\Omega, \mathcal{L}Y\Omega), \tag{2}$$

for all $X, Y \in \mathfrak{U}$. The required flow is then given by $\sigma^t(X) = \mathrm{e}^{i\mathcal{L}t}X\mathrm{e}^{-i\mathcal{L}t}$ (see [GP] for a proof of this fact). I shall say that σ is the modular group and $\mathcal{L}$ the modular generator of $\mathcal{S}$. From the definition (2), a number of important properties of $\mathcal{L}$ are easily obtained:

- ▶ $\mathcal{L}$ is a derivation: $\mathcal{L}XY\Omega = X\mathcal{L}Y\Omega + Y\mathcal{L}X\Omega$.
- ▶ In particular: $\mathcal{L}\Omega = 0$.
- ▶ $[L, \mathcal{L}] = 0$.
- ▶ The modular group is symplectic: $[\mathcal{L}, \{X, Y\}] = \{[\mathcal{L}, X], Y\} + \{X, [\mathcal{L}, Y]\}$.

For the finite system of example 2, the state ω is regular if it is given by a measure of the form $d\mu = \mathrm{e}^{\varphi}d\ell$, where φ is smooth enough to generate a Hamiltonian flow Φ_φ. Then the modular group is $\sigma^t(X) = X \circ \Phi^t_\varphi$ and $\mathcal{L} = i\{\varphi, \cdot\}$. Note also that $\mathcal{S}$ is at thermal equilibrium at inverse temperature β, if and only if it is in a regular state and

$$\mathcal{L} = -\beta L.$$

Remark 10 If the system decomposes into non-interacting subsystems, $\sum_\alpha \mathcal{S}_\alpha$, its modular structure factorizes in a simple way: $J = \otimes_\alpha J_\alpha$ in the quantum case and $\mathrm{e}^{\mathcal{L}t} = \otimes_\alpha \mathrm{e}^{\mathcal{L}_\alpha t}$ in both, the classical and the quantum case. In particular, if all subsystems are at thermal equilibrium, with possibly different temperatures, the modular generator is given by

$$\mathcal{L} = -\sum_\alpha \beta_\alpha L_\alpha.$$

4 Far from equilibrium

I shall consider a simple class of models where a «small» system Σ, with a finite number of degrees of freedom, is driven away from equilibrium by reservoirs $\mathcal{R}_1, \cdots, \mathcal{R}_n$ in thermal equilibrium at inverse temperatures $\beta_1, \cdots, \beta_n$. Let me denote by $\mathcal{S}$ the uncoupled system $\Sigma + \sum_{\alpha=1}^n \mathcal{R}_\alpha$. Its normal form is given by

$$\begin{array}{rcl} \mathcal{H} & = & (\otimes_{\alpha=1}^n \mathcal{H}_\alpha) \otimes \mathcal{H}_\Sigma, \\ \Omega & = & (\otimes_{\alpha=1}^n \Omega_\alpha) \otimes \Omega_\Sigma, \\ \mathfrak{M} & = & (\otimes_{\alpha=1}^n \mathfrak{M}_\alpha) \otimes \mathfrak{M}_\Sigma, \\ L & = & (\sum_{\alpha=1}^n L_\alpha) + L_\Sigma. \end{array}$$

The modular generator of $\mathcal{S}$ is

$$\mathcal{L} = \sum_{\alpha=1}^n \mathcal{L}_\alpha + \mathcal{L}_\Sigma,$$

where

$$\mathcal{L}_\alpha = -\beta_\alpha L_\alpha. \tag{3}$$

In the quantum case, the modular conjugation is $J = (\otimes_{\alpha=1}^n J_\alpha) \otimes J_\Sigma$. The coupling of Σ with the reservoirs is described by the interaction $V = \sum_{\alpha=1}^n V_\alpha$, where $V_\alpha = V_\alpha^* \in \mathfrak{M}_\alpha \otimes \mathfrak{M}_\Sigma$. In the quantum case, the dynamics is defined by

$$\tau_V^t(X) = \mathrm{e}^{-i(L+V)t} X \mathrm{e}^{i(L+V)t}.$$

In the classical case, the existence of the coupled dynamics is a more delicate question which I will not consider here (see however Section 3 in [JP1] for a soft approach to this problem). I assume that the Hamiltonian $H_V \equiv \sum_{\alpha=1}^n H_\alpha + H_\Sigma + V$ induces a global flow Φ_V^t on phase space, *i.e.*, that the operator

$$L_V \colon X\Omega \mapsto LX\Omega + i\{V, X\}\Omega,$$

generates a strongly continuous group on $\mathcal{H}$. Then

$$\tau_V^t(X) \equiv X \circ \Phi_V^t = \mathrm{e}^{iL_V t} X \mathrm{e}^{-iL_V t},$$

defines the dynamics on $\mathfrak{M}$.

In both, classical and quantum case, I also assume that for some normal faithful state ν of $\mathcal{S}$

$$\nu_V^+(X) \equiv \lim_{t\to+\infty} \nu \circ \tau_V^t(X), \tag{4}$$

defines a natural nonequilibrium state on some subalgebra $\mathfrak{U}^+ \subset \mathfrak{M}$ containing $\mathfrak{M}_\Sigma$. Finally, I need a more technical regularity assumption on the interaction,

$$i[\mathcal{L}, V] \in \mathfrak{U}^+. \tag{5}$$

Note that, at the current level of generality, the existence of the limit (4) is a very challenging mathematical problem (see [EPR1] and [JP3] for simpler examples).

4.1 Relative entropy and entropy production

In the study of thermostated systems, the rate of phase space contraction and its relation to entropy production play an important role. Since we are dealing with infinite dimensional Hamiltonian systems, it is not clear what remains of this relation in our model. I will start with a discussion of classical systems, and then proceed by analogy to the quantum case.

4.1.1 Classical systems

Using the definition (2) and the properties of the modular generator $\mathcal{L}$, one easily gets the formula

$$L_V^* = L_V + i\sigma_V,$$

where $\sigma_V \equiv i[\mathcal{L}, V]$ is an observable (the derivative of V along the modular group). It immediately follows that

$$J_V^t \equiv \mathrm{e}^{-iL_V^* t} \mathrm{e}^{iL_V t} = \mathrm{e}^{\int_0^t \tau_V^{-s}(\sigma_V) ds}.$$

From the fact that $L_V \Omega = 0$, we further get

$$\omega \circ \tau_V^t(X) = (\Omega, \mathrm{e}^{iL_V t} X \mathrm{e}^{-iL_V t}\Omega) = (\Omega, \mathrm{e}^{-iL_V^* t} \mathrm{e}^{iL_V t} X\Omega) = \omega(J_V^t X),$$

which shows that J_V^t is the Radon-Nikodym derivative

$$J_V^t = \frac{d\omega \circ \tau_V^t}{d\omega}.$$

Let us now start the system in an arbitrary normal state ω_0. Computing the relative entropy of the state at time t, $\omega_t \equiv \omega_0 \circ \tau_V^t$, with respect to our reference state ω, we obtain

$$S(\omega_t|\omega) \equiv -\omega_t(\log \frac{d\omega_t}{d\omega}) = S(\omega_0|\omega) - \int_0^t \omega_s(\sigma_V)ds. \tag{6}$$

It is therefore natural to define the entropy production rate in the state μ, as

$$e_V(\mu) \equiv \mu(\sigma_V).$$

Since by assumption (5) the limit (4) exists on σ_V, we get

$$\lim_{t\to+\infty} \frac{S(\nu|\omega) - S(\nu_t|\omega)}{t} = e_V(\nu_V^+).$$

Furthermore, the fact that $S(\cdot|\omega)$ is bounded above, shows that the entropy production is non-negative in a natural equilibrium state

$$e_V(\nu_V^+) \geq 0.$$

Proving strict positivity of the entropy production is another challenging mathematical problem (see [EPR2] for an example).

4.1.2 Quantum systems

Since there is no natural way to define phase space contraction in quantum mechanics, I proceed directly to the computation of relative entropy. Let μ, ν be two faithful normal states, their relative entropy is defined by

$$S(\mu|\nu) \equiv (\Omega_\mu, \log \Delta_{\nu|\mu}\Omega_\mu),$$

where Ω_μ is the unique vector representative of the state μ in the natural cone $\mathcal{P}$ and $\Delta_{\nu|\mu}$ is the relative modular operator. To compute the relative entropy $S(\omega_t|\omega)$ of the state $\omega_t \equiv \omega_0 \circ \tau_V^t$ with respect to the reference state ω, we use the following simple facts:

1. If $U \in \mathfrak{M}$ is unitary, then the vector representative of the state $\psi_U(X) \equiv \omega(U^*XU)$ is $Uj(U)\Omega \in \mathcal{P}$. Moreover the relative modular operators are given by $\Delta_{\psi_U|\omega} = U\mathrm{e}^{\mathcal{L}}U^*$ and $\Delta_{\omega|\psi_U} = j(U)\mathrm{e}^{\mathcal{L}}j(U^*)$.
2. $\tau_V^t(X) = \tau^t(U_t^*XU_t)$, where τ^t is the non-interacting dynamics and $U_t \equiv \mathrm{e}^{-i(L+V)t}\mathrm{e}^{iLt}$ is a unitary element of $\mathfrak{M}$.

The result is again expressed by formula (6), with $\sigma_V \equiv i[\mathcal{L}, V]$. Since the quantum relative entropy is non-positive, we can repeat the argument of the previous subsection to prove $e_V(\nu_V^+) \geq 0$.

4.2 Heat flows

We expect the non-equilibrium state ν_V^+ to describe steady heat currents Φ_α, flowing from $\mathcal{R}_\alpha$ into the small system Σ. Formally, we would like to define Φ_α by $\tau_V^t(\Phi_\alpha) = \partial_t\tau_V^t(H_\alpha)$, where H_α is the energy of $\mathcal{R}_\alpha$. Since this quantity is not observable we set

$$\partial_t\tau_V^t(H_\Sigma + V) = -\sum_{\alpha=1}^{n}\tau_V^t(\Phi_\alpha),$$

where $\Phi_\alpha \in \mathfrak{M}_\Sigma \otimes \mathfrak{M}_\alpha$. Note that Φ_α is positive when energy is flowing from Σ into $\mathcal{R}_\alpha$. A simple calculation leads to the formula

$$\Phi_\alpha = -i[L_\alpha, V_\alpha].$$

Since by definition $\sum_\alpha \Phi_\alpha$ is a total derivative, we have in the stationary state

$$\sum_{\alpha=1}^{n}\nu_V^+(\Phi_\alpha) = 0. \tag{7}$$

On the other hand, using (3), we get

$$\sigma_V = i[\mathcal{L}, V] = \sum_{\alpha=1}^{n}\beta_\alpha\Phi_\alpha + i[\mathcal{L}_\Sigma, V],$$

where the last term can be further expressed as $i[\mathcal{L}_\Sigma, L+V]$, which is also a total derivative. Hence, assuming $\Phi_\alpha \in \mathfrak{M}^+$, we can relate entropy production to the usual phenomenological expression for the entropy flux

$$\sum_{\alpha=1}^{n}\beta_\alpha\nu_V^+(\Phi_\alpha) = e_V(\nu_V^+), \tag{8}$$

As a final remark, note that for $n = 2$, the formulae (7) and (8) combine to

$$(\beta_1 - \beta_2)\nu_V^+(\Phi_1) = e_V(\nu_V^+) \geq 0,$$

which means that heat flows from the hot reservoir to the cold one.

References

[A1] M. AIZENMAN, G. GALLAVOTTI, S. GOLDSTEIN, J.L. LEBOWITZ: Stability and equilibrium states of infinite classical systems. *Commun. Math. Phys.,* 48 (1976), 1–14.

[A2] M. AIZENMAN, S. GOLDSTEIN, C. GRUBER, J.L. LEBOWITZ, PH. MARTIN: On the equivalence between KMS-states and equilibrium states for classical systems. *Commun. Math. Phys.,* 53 (1977), 209–220.

[AWo] H. ARAKI, E.J. WOODS: Representation of the canonical commutation relations describing a non-relativistic infinite free Bose gas. *J. Math. Phys.,* 4 (1963), 637–662.

[AWy] H. ARAKI, W. WYSS: Representation of canonical anticommutation relations. *Helv. Phys. Acta,* 37 (1964), 139–159.

[BFS] V. BACH, J. FRÖHLICH, I.M. SIGAL: Return to equilibrium. Preprint 1999. Available on mp_arc, preprint #99-485.

[BR1] O. BRATTELI, D.W. ROBINSON: *Operator Algebras and Quantum Statistical Mechanics 1.* Springer, New York, 1979.

[BR2] O. BRATTELI, D.W. ROBINSON: *Operator Algebras and Quantum Statistical Mechanics 2.* Springer, New York, 1981.

[CG] E.G.D. COHEN, G. GALLAVOTTI: Dynamical ensembles in stationary states. *J. Stat. Phys.,* 80 (1995), 931–970.

[DJ] J. DEREZINSKI, V. JAKŠIĆ: Spectral theory of Pauli-Fierz Hamiltonians I. Preprint 1998. Available on mp_arc, preprint #98-755.

[DJP] J. DEREZINSKI, V. JAKŠIĆ, C.-A. PILLET: Spectral theory of Pauli-Fierz Hamiltonians II. In preparation.

[EPR1] J.-P. ECKMANN, C.-A. PILLET, L. REY-BELLET: Non-equilibrium statistical mechanics of anharmonic chains coupled to two heat baths at different temperatures. *Commun. Math. Phys.,* 201 (1999), 657–697.

[EPR2] J.-P. ECKMANN, C.-A. PILLET, L. REY-BELLET: Entropy production in non-linear, thermally driven Hamiltonian systems. *J. Stat. Phys.,* 95 (1999), 305–331.

[EH] J.-P. ECKMANN, M. HAIRER: Nonequilibrium statistical mechanics of strongly anharmonic chains of oscillators. Preprint 1999. Available on mp_arc, preprint #99-356.

[FL] F. FIDALEO, C. LIVERANI: Ergodic properties for a quantum nonlinear dynamics. *J. Stat. Phys.,* 97 (1999), 957–1009.

[GP] G. GALLAVOTTI, M. PULVIRENTI: Classical KMS condition and Tomita-Takesaki theory. *Commun. Math. Phys.,* 97 (1976), 1–9.

[JP1] V. JAKŠIĆ, C.-A. PILLET: Ergodic properties of classical dissipative systems I. *Acta Math.,* 181 (1998), 245–282.

[JP2] V. JAKŠIĆ, C.-A. PILLET: On a model for quantum friction III. Ergodic properties of the spin-boson system. *Commun. Math. Phys.,* 178 (1996), 627–651.

[JP3] V. JAKŠIĆ, C.-A. PILLET: Natural nonequilibrium state of N-level systems. In preparation.

[RT] L. REY-BELLET, L.E. THOMAS: Asymptotic behavior of thermal nonequilibrium steady states for a driven chain of anharmonic oscillators. Preprint 2000. Available on mp_arc, preprint #00-8.

[R1] D. RUELLE: What are the Measures Describing Turbulence? *Prog. Theor. Phys.,* 64 (1978), 339–345.

[R2] D. RUELLE: Positivity of entropy production in nonequilibrium statistical mechanics. *J. Stat. Phys.,* 85 (1996), 1–23.

[R3] D. RUELLE: Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics. *J. Stat. Phys.,* 95 (1999), 393–468.

[R4] D. RUELLE: Natural nonequilibrium states in quantum statistical mechanics. Preprint 1999. Available on mp_arc, preprint #00-12.

[R5] D. RUELLE: A Remark on the equivalence of isokinetic and isoenergetic thermostats in the thermodynamic limit. Preprint 2000. Available on mp_arc, preprint #00-29.